Supplementary Information for:

The Reaction Mechanism with Free Energy Barriers for Electrochemical dihydrogen Evolution on MoS_2

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S1 – Free Energy Barrier from Experimental Estimate

From [1], the experimental turnover frequency (TOF) is estimated to be 1.64 x 10^{-2} s^{-1} per edge Mo atom on the $(10\bar{1}0)$ Mo-edge. Since the MoS_2 used in this study models the 3-Mo wide segment of the edge, we have TOF ≈ (k_BT/h) × exp(-$\Delta G^{\ddagger}$/RT). Using k_B = 1.38 x 10^{-23} m^2 kg s^{-2} K^{-1}, T = 298K, h = 6.63 x 10^{-34} J·s, R = 1.987 x 10^{-3} kcal/(K·mol), $\Delta G^{\ddagger}$ is found to be 19.9 kcal/mol.

S2 – Geometries of Relevant Structures [Unit: Angstroms]

[MoS_2]

E = -9039.45984 Hartree

Mo1	1.7834476948	0.4270694692	6.2545498501
S2	-0.2453984236	1.5345934647	6.2659886554
Mo3	1.6426038211	3.1337395274	6.2527065206
S4	0.0113974890	4.9245860916	6.2446643344
Mo5	1.7829950284	6.5792589857	6.2481686019
S6	0.0293374628	8.3222490382	6.2613222882
Mo7	2.1404525150	9.2654614914	6.2419870243
S8	3.6539478318	-0.9288601128	6.2386066188
S9	2.5961634902	1.7289642990	4.5054505441
S10	2.6180514640	1.7295595975	7.9916589268
Mo11	4.2903390411	1.4614001981	6.2377973385
S12	2.6035416962	4.8184158295	4.7226021502
S13	2.6223607558	4.8220525604	7.7650879780
Mo14	4.5156453171	4.7465777189	6.2315492904
S15	2.8485985447	7.8973909006	4.4979356550
S16	2.8702501294	7.9049995491	7.9823469219
Mo17	4.5580544404	8.0364288679	6.2289632623
S18	6.6083543583	0.7550709936	6.2188258048

S19	5.3894573781	3.0607869529	4.7087768926
S20	5.4089310424	3.0650365471	7.7479283136
Mo21	7.3467423384	3.0639231311	6.2165470591
S22	5.5266166540	6.3531974872	4.7041163053
S23	5.5462581622	6.3557520414	7.7435211470
Mo24	7.4765071225	6.1934350220	6.2121383483
S25	4.1130889256	10.4685376890	6.2265863935
S26	9.6728090564	2.2263644970	6.2071635223
S27	8.0707652040	4.5994157918	4.4673152297
S28	8.0963459897	4.6030437479	7.9516148702
Mo29	9.6228806088	4.5371191424	6.1982635896
S30	6.9258984530	8.5543958828	6.2059894935
S31	9.8631330503	6.8363423297	6.2010069968

$[MoS_2]^-$

E = -9039.58867 Hartree

Mo1	1.7825913344	0.4264638817	6.2525433187
S2	-0.2450295305	1.4833088400	6.2723195398
Mo3	1.6612863574	3.1417977298	6.2500779055
S4	0.0393587418	4.9206143071	6.2608845829
Mo5	1.8017670052	6.5710099705	6.2451067625
S6	0.0357693740	8.3687245269	6.2622701521
Mo7	2.1401161878	9.2672637553	6.2402926285
S8	3.6707383562	-0.9328489608	6.2507641976
S9	2.5788696059	1.7182795891	4.4819437246
S10	2.6014677676	1.7227921016	8.0095056226
Mo11	4.2783788775	1.4554402685	6.2359565675
S12	2.6008756058	4.8185178438	4.7018333732
S13	2.6203703540	4.8220358806	7.7819967094

Mo14	4.5119164884	4.7464197697	6.2299579629
S15	2.8320405005	7.9100488984	4.4740517519
S16	2.8530065675	7.9131774921	8.0010088980
Mo17	4.5454052655	8.0438476550	6.2278255205
S18	6.6354923858	0.7599906207	6.2208954738
S19	5.3809261065	3.0548193146	4.7091894295
S20	5.3992302662	3.0588450385	7.7445595405
Mo21	7.3352823458	3.0559797160	6.2156110078
S22	5.5176874191	6.3602794545	4.7055679715
S23	5.5357470854	6.3622334814	7.7404300395
Mo24	7.4651637531	6.2027158067	6.2120207684
S25	4.1329713160	10.4703894251	6.2356955162
S26	9.7070769646	2.2380319527	6.2097445196
S27	8.0644320800	4.6000302893	4.4663417423
S28	8.0863132638	4.6032706779	7.9526451448
Mo29	9.6152940670	4.5375317209	6.1996992418
S30	6.9535974083	8.5459311835	6.2133222248
S31	9.8977635870	6.8210006653	6.2051213434

Transition state from **$[MoS_2]^-$** to **$[MoS_2]H_S$**

E = -9345.86587 Hartree

Mo1	1.5804130204	0.6261952888	6.1641263706
S2	-0.3238753399	1.7746540555	5.5115805215
Mo3	1.6041837582	3.2981264477	5.7279660888
S4	0.1326678915	5.1110725795	5.0368138436
Mo5	1.9389946694	6.6900154067	5.2477870841
S6	0.3250944668	8.4717285632	4.6101328527
Mo7	2.4329909633	9.3349240700	4.9257259091
S8	3.2796033079	-0.7572597913	6.8572071909

S9	2.8833462495	1.6168381911	4.5117967071
S10	2.0234545738	2.1711239499	7.8479130019
Mo11	4.0684261532	1.6008246675	6.6453800737
S12	3.0175205320	4.6984063424	4.2627053439
S13	2.2776101996	5.1842460546	7.1724119189
Mo14	4.4855648565	4.8376790477	6.2012708626
S15	3.4836423367	7.7034478561	3.6437136416
S16	2.6338330324	8.2523417322	6.9824260087
Mo17	4.7008637058	8.0813181252	5.7101124277
S18	6.2327549826	0.8352472680	7.3234408789
S19	5.6154750660	2.9097644215	5.2333546996
S20	4.8633345082	3.4022186845	8.1339563855
Mo21	7.1203935641	3.1182124157	7.1808099691
S22	5.9419312285	6.1548100229	4.7477392262
S23	5.2058355497	6.6713628130	7.6679926003
Mo24	7.4366994758	6.1514821604	6.7340815799
S25	4.3863118536	10.5049217687	5.3736167793
S26	9.2533817441	2.2089765789	7.9730824467
S27	8.4001057175	4.3160147149	5.4477475969
S28	7.4971214715	4.9043132057	8.8255236549
Mo29	9.4073816516	4.4769514139	7.5469795646
S30	7.0751125781	8.5539574426	6.0734723368
S31	9.7727154591	6.7502075353	7.3116477782
O32	8.2784963303	7.8150012411	11.3491016065
H33	7.3190737121	7.9623320030	11.1463106204
H34	8.3915960702	8.0009597275	12.2890428932
H35	9.0460842541	8.7479806707	10.2945597635
O36	9.3370840273	9.3192362802	9.5150815158
H37	9.7987651579	8.7154393986	8.9073555331

H38	8.1790627985	9.7547792006	8.9364337156
O39	5.8115760406	8.4781400717	10.5193839361
H40	5.3417081335	7.7738511657	10.0488394437
H41	6.0563248527	9.1166521603	9.8262471805
O42	7.2056243670	10.0216030172	8.5139017657
H43	7.1040459230	9.4104108960	7.4200987100
H44	7.1762675495	10.9743456626	8.3379660727

$[MoS_2]H_s$

E = -9040.04750 Hartree

Mo1	1.7829884959	0.4383747584	6.3265523463
S2	-0.2411220540	1.5197293533	6.3394612416
Mo3	1.6567595219	3.1509102497	6.2933155066
S4	0.0230286296	4.8841723414	6.3042239899
Mo5	1.7911309442	6.5956098589	6.2484220288
S6	0.0009667099	8.2561725089	6.3060050359
Mo7	2.0960739073	9.2561496160	6.2162831532
S8	3.6776077779	-0.9101375098	6.3099832387
S9	2.5802939050	1.7167528463	4.5515399143
S10	2.6338206662	1.7606140915	8.0431812017
Mo11	4.2836178722	1.4665802213	6.2743656785
S12	2.6034378275	4.8192080915	4.7358623772
S13	2.6617267695	4.8599992801	7.7700385463
Mo14	4.5374796079	4.7740438763	6.2183505609
S15	2.7968599600	7.9198026339	4.4297723159
S16	2.8850147975	7.9467583731	7.9873290532
Mo17	4.5060607538	8.0343397984	6.1649565686
S18	6.6328407376	0.7641691740	6.2581181599
S19	5.3713617188	3.0486592248	4.7164456015

S20	5.4125102542	3.0987061002	7.7515783611
Mo21	7.3357529054	3.0463655054	6.2113009537
S22	5.5343952361	6.3525649918	4.6374337926
S23	5.6106422474	6.4280831498	7.6964986088
Mo24	7.5112678159	6.1684318888	6.1514178308
S25	4.0545125309	10.4620991645	6.2072487120
S26	9.6953877566	2.2089094998	6.2428809310
S27	8.0663201060	4.5559812636	4.4369512557
S28	8.0980829679	4.5998551830	7.9149960081
Mo29	9.6275375767	4.4946543082	6.1623012767
S30	6.9841576071	8.6209952411	5.8331717310
S31	9.8552602383	6.8189851065	6.2722298794
H32	7.4137973344	9.1162263380	7.0112243530

$[MoS_2]H_s^-$

E = -9040.17167 Hartree

Mo1	1.7878860830	0.4336741657	6.3300284623
S2	-0.2431786599	1.5187294307	6.3472878402
Mo3	1.6590613912	3.1421672584	6.2962264152
S4	0.0254908788	4.9011806860	6.3049805999
Mo5	1.7886407762	6.5798613092	6.2468083987
S6	0.0011986871	8.2904343068	6.2833065075
Mo7	2.0930203486	9.2555462078	6.2119013534
S8	3.6412633181	-0.9344024490	6.3242865654
S9	2.5846087118	1.7110863161	4.5444389292
S10	2.6360181968	1.7584553310	8.0574722999
Mo11	4.2907161646	1.4769408093	6.2799796769
S12	2.6007599718	4.8076242437	4.7371562582
S13	2.6544297628	4.8507582153	7.7750006605

Mo14	4.5355620237	4.7770029262	6.2252352977
S15	2.8080500656	7.8927865954	4.4384713078
S16	2.8975142463	7.9266926465	7.9708016050
Mo17	4.5101367883	8.0506591207	6.1605255959
S18	6.5855252469	0.7560680559	6.2626471850
S19	5.3812035093	3.0515555488	4.7214729015
S20	5.4222263794	3.1018807952	7.7560982254
Mo21	7.3452038861	3.0664506594	6.2133630739
S22	5.5346454483	6.3675241114	4.6415914736
S23	5.6073848721	6.4576634626	7.6968465849
Mo24	7.5044927772	6.1559824640	6.1481450734
S25	4.0772737307	10.4559494519	6.1880355144
S26	9.6607927217	2.1887598328	6.2156931233
S27	8.0823890082	4.5631966086	4.4120816327
S28	8.0990358793	4.6309958369	7.9435098554
Mo29	9.6315172877	4.4915531787	6.1739593535
S30	6.9682479313	8.6216908625	5.8993239586
S31	9.8624397262	6.8001486932	6.1633583891
H32	7.2865641812	9.1128980877	7.1124814257

Transition state from **$[MoS_2]H_S^-$** to **$[MoS_2]H_{Mo}^-$**

E = -9040.15721 Hartree

Mo1	1.6636329342	1.0689983114	7.8923050354
S2	-0.3254318610	2.1724719052	7.5594782166
Mo3	1.6358435685	3.6060843010	6.9139926827
S4	0.0749722088	5.3264262315	6.3401501426
Mo5	1.9244241392	6.8095603915	5.6596263160
S6	0.2178940314	8.4684632875	5.0481411043
Mo7	2.3716213727	9.2739750166	4.6944633545

S8	3.4413520061	-0.3254286691	8.3368132971
S9	2.4594387918	1.6059113959	5.7727785093
S10	2.6238289414	2.8625930106	9.0220416400
Mo11	4.2175132908	1.8860815417	7.4446515740
S12	2.6060398137	4.5734644341	4.8636814865
S13	2.7441437033	5.6679651146	7.6917647447
Mo14	4.5728048444	4.9318164519	6.2527880848
S15	2.9389602186	7.3415017098	3.4932949715
S16	3.1438513738	8.6375528438	6.7933104536
Mo17	4.7345093096	7.9711546587	5.0840210912
S18	6.4702702607	1.0741389526	7.6209557834
S19	5.3170070083	2.7670943584	5.4194365399
S20	5.4621991509	3.8546401971	8.2525765469
Mo21	7.3309963249	3.2148721999	6.7770469252
S22	5.5757694315	5.8268191041	4.2075226345
S23	5.7273701593	6.9200745642	7.0822743659
Mo24	7.5537870934	6.1123998144	5.6557164559
S25	4.3238501460	10.2593507102	4.0624565475
S26	9.5994974612	2.2954596453	7.0419133606
S27	8.0467020252	3.9934509602	4.5519325673
S28	8.2223418635	5.2369548095	7.8529396091
Mo29	9.6477521855	4.4549821456	6.1802126296
S30	7.2300558591	8.2835303180	4.7256389358
S31	10.0346372830	6.5688987549	5.4173408976
H32	6.1618098982	9.0268278061	5.6481196571

$[MoS_2]H_{Mo}^-$

E = -9040.16238 Hartree

Mo1	1.7867850409	0.4391737914	6.2343940787

S2	-0.2542715888	1.5130178235	6.2513286819
Mo3	1.6400883361	3.1497613646	6.2443444829
S4	-0.0019669536	4.9105335772	6.2366564458
Mo5	1.7785262478	6.5894632310	6.2421435629
S6	0.0133227071	8.3168431638	6.2462533898
Mo7	2.1361363809	9.2682777240	6.2132182894
S8	3.6151077532	-0.9477185214	6.2166182542
S9	2.5998415240	1.7461261773	4.4886648874
S10	2.6206371939	1.7347009350	7.9789029439
Mo11	4.3025553741	1.4771055636	6.2264256783
S12	2.6159758632	4.8326678867	4.7290267248
S13	2.6089381858	4.8339046878	7.7677722816
Mo14	4.5196439987	4.7626833557	6.2523554165
S15	2.8688868634	7.8997033002	4.4804222341
S16	2.8435307780	7.9376944651	7.9887780203
Mo17	4.5674358753	8.0260109624	6.2363946917
S18	6.5673103475	0.7295875068	6.2227187974
S19	5.4027599028	3.0932291565	4.7149274896
S20	5.4198907189	3.0632797317	7.7511999881
Mo21	7.3632097648	3.0688278931	6.2121554724
S22	5.5605837688	6.3593121680	4.7340910032
S23	5.5167491322	6.3770212023	7.8005242345
Mo24	7.4701748327	6.1734163022	6.3103809029
S25	4.0172816444	10.5393359722	6.2462426630
S26	9.6332722265	2.1596568449	6.0907017111
S27	8.1280784848	4.5995683881	4.4652594710
S28	8.1206185501	4.5812877804	8.0010748353
Mo29	9.6439782727	4.4886666211	6.2505257749
S30	6.8060511472	8.6295499019	6.1055491958

S31	9.9775997361	6.7186999544	6.0345634386
H32	8.0314869309	7.1231955979	7.6014052975

Transition state from **$[MoS_2]H_{Mo}^-$** to **$[MoS_2]H_SH_{Mo}$**

E = -9346.44512 Hartree

Mo1	1.6071162552	0.6053280881	6.0396619200
S2	-0.2937065588	1.7580095029	5.3739325528
Mo3	1.6184140991	3.2840780540	5.6550816644
S4	0.1491197305	5.1037535299	4.9595181759
Mo5	1.9354555972	6.6860624050	5.2430138897
S6	0.3260660497	8.4702119396	4.5887102850
Mo7	2.4184297030	9.3400270129	4.9699967653
S8	3.3052816928	-0.7819773972	6.7180543363
S9	2.9270051461	1.6364854654	4.4250700460
S10	2.0154371210	2.1201111900	7.7588263080
Mo11	4.0808918838	1.5908406574	6.5786654459
S12	3.0553839489	4.7249349097	4.2523463174
S13	2.2412203707	5.1486298500	7.1512230237
Mo14	4.4775712243	4.8439901336	6.2308834874
S15	3.5214412604	7.7340699588	3.7029632343
S16	2.5595580577	8.2292225894	7.0156022044
Mo17	4.6766305101	8.0940490940	5.8046442696
S18	6.2221205660	0.8196446656	7.2894991091
S19	5.6337734289	2.9545469059	5.2197004404
S20	4.8425044271	3.3553177034	8.1287963647
Mo21	7.1176324554	3.1098259442	7.1793522574
S22	5.9617938534	6.1950097513	4.8608312620
S23	5.1286994089	6.6553217527	7.7544263300
Mo24	7.3966004505	6.1875837160	6.9011300546
S25	4.3239299227	10.5311953990	5.5274036621

S26	9.2685279668	2.1379787631	7.7998987076
S27	8.4153165521	4.3544381857	5.5204535535
S28	7.4651988763	4.8400612584	8.8936597548
Mo29	9.3892170748	4.4488539771	7.6533148819
S30	7.0342296785	8.6024218848	6.0957024015
S31	9.9037097652	6.6301906444	7.2260502734
O32	8.2451667515	7.8610942127	11.2472967584
H33	7.2979814090	8.0807869665	11.0511487323
H34	8.3788828168	8.0464269636	12.1847355769
H35	9.0782129068	8.7301638027	10.1807746493
O36	9.4081598682	9.2757685141	9.3997082377
H37	9.8201822705	8.6377163534	8.7917752286
H38	8.2754757730	9.8102966310	8.8446816282
O39	5.8163770846	8.6991862475	10.4470630644
H40	5.3140543265	8.0112991114	9.9854237025
H41	6.1083335682	9.3093524846	9.7460262909
O42	7.3180870912	10.1570358437	8.4538914295
H43	7.1250447868	9.5295185807	7.3668162035
H44	7.3617701282	11.1076553328	8.2712607860
H45	7.6555754872	7.2715694697	8.1769078716

$[MoS_2]H_SH_{Mo}$

E = -9040.62797 Hartree

Mo1	1.7994828409	0.4318836549	6.2854072329
S2	-0.2350758428	1.5635952355	6.2784538075
Mo3	1.6503797939	3.1302177990	6.2626792211
S4	0.0071926327	4.9522522240	6.2547163057
Mo5	1.7671093521	6.5652232302	6.2246479724
S6	0.0024122397	8.3401308796	6.2611708723

Mo7	2.1008615796	9.2551779989	6.1863120963
S8	3.6424669922	-0.9306563962	6.2822503330
S9	2.6106999444	1.7197713426	4.5243071437
S10	2.6275529160	1.7509216852	8.0150301246
Mo11	4.3051012954	1.4837829572	6.2647784710
S12	2.6182215204	4.8031990348	4.7246206439
S13	2.6249392459	4.8374999573	7.7636669115
Mo14	4.5285452703	4.7747101845	6.2426295357
S15	2.8392474060	7.8765986195	4.4617942188
S16	2.8176089991	7.9095165944	7.9475165873
Mo17	4.5157063312	8.0466557722	6.1945632230
S18	6.5676530091	0.7500799477	6.2586218571
S19	5.4034469237	3.0798211199	4.7294530457
S20	5.4193855888	3.0980546725	7.7683823463
Mo21	7.3601918686	3.0857734344	6.2288089846
S22	5.5459498973	6.3410688047	4.6930045096
S23	5.5322663801	6.4381720707	7.7496004316
Mo24	7.4854985768	6.1790564418	6.2630237815
S25	4.0916577947	10.4505142235	6.3767589406
S26	9.6056341366	2.1583441712	6.1242612662
S27	8.1394694842	4.5709080168	4.4452665533
S28	8.1179071933	4.6309400509	7.9931717922
Mo29	9.6420484153	4.4838337454	6.2456310711
S30	6.9063877990	8.6448659127	5.7254655472
S31	9.9758426802	6.7061230561	5.9727733812
H32	7.1844895975	9.3860820498	6.8157229315
H33	8.0477625181	7.1522683153	7.5331172814

Heyrovsky transition state from **[MoS_2]H_SH_{Mo}**

E = -9346.81634 Hartree

Mo1	1.7979251529	0.4655188303	5.7061460768
S2	-0.1772433388	1.4749588317	6.3128139410
Mo3	1.7209461478	3.0935656306	6.3791400916
S4	0.1412098233	4.7502718228	7.0775116272
Mo5	1.9181026836	6.4371269424	7.1935586386
S6	0.2073436122	8.0120105047	7.9750485469
Mo7	2.2831244381	9.0264642905	7.7886329044
S8	3.6076209595	-0.8044284862	5.0251908015
S9	2.3236319781	2.1666525437	4.2065504399
S10	2.9485282667	1.3271593279	7.5353433391
Mo11	4.2838327115	1.5243840789	5.5055371344
S12	2.4427187675	5.1267735748	5.1713010133
S13	2.9737668777	4.3845997176	8.0676196112
Mo14	4.5845611801	4.7254441520	6.2742482079
S15	2.6708148115	8.2055280297	5.6405823826
S16	3.2796753033	7.3156473482	9.0335144951
Mo17	4.6271239312	7.8775205395	7.0612044831
S18	6.5405439283	0.8790331691	4.9156094556
S19	5.1171934138	3.4860325148	4.2471495224
S20	5.6904065129	2.7295557955	7.1378442607
Mo21	7.3099681435	3.1441648472	5.3065283691
S22	5.3711285418	6.6540692321	5.0293560074
S23	5.8839201333	5.9381474425	7.9448140044
Mo24	7.5742085761	6.1521418778	6.1490723072
S25	4.2579833594	10.2038719362	7.8640332327
S26	9.4920703386	2.3843330228	4.4532812839
S27	7.7619103385	5.1101014359	3.9271303547

S28	8.4534741522	4.1344334881	7.2114634838
Mo29	9.6094591154	4.5524825944	5.2418616781
S30	6.9476778282	8.6558114628	6.3107413040
S31	9.9809548731	6.7817505502	5.4723676723
H32	8.5176246930	6.8841136599	7.5938637351
O33	5.2276914323	5.6386244644	11.8846449647
H34	5.9829643002	6.9680224132	11.3834754358
H35	5.1565512708	5.4349681082	12.8246032297
H36	5.7375427550	4.9009332718	11.4663582244
O37	6.8553230367	3.9417546459	10.5643278838
H38	6.4270962182	3.5507647483	9.7892813007
H39	7.4809416694	4.5924040732	10.2024235708
O40	6.5218169129	7.6774277925	10.9141718263
H41	5.9138427939	8.0782036147	10.2759968471
H42	7.6213251129	6.9950277202	10.2619860511
O43	8.3913605685	6.4299950626	9.8146083124
H44	8.4250645628	6.6501580761	8.4637960534
H45	9.2337205115	6.6833536602	10.2197465074
H46	7.5402024146	9.0587898011	7.4524155837

Heyrovsky transition state from **$[MoS_2]H_S^-$**

E = -9346.39453 Hartree

Mo1	1.8856686449	0.3795580790	6.4880447161
S2	-0.1030685717	1.4433445927	6.9872910562
Mo3	1.7381033370	3.0846084977	6.7221342942
S4	0.1592750582	4.8730545435	7.1590136992
Mo5	1.9284400545	6.5508208927	6.9266137746
S6	0.2460884633	8.3085255835	7.3355980076
Mo7	2.3501757835	9.2348875663	7.0169703874

S8	3.7037813900	-0.9539329783	5.9834774437
S9	2.3305796443	1.8176784243	4.7179049729
S10	3.0569373940	1.5614564904	8.1106636174
Mo11	4.3512013505	1.4374475683	6.0427885292
S12	2.3702451299	4.8812609352	5.1633271642
S13	2.9750994758	4.6666944459	8.1412942618
Mo14	4.5302188133	4.6774998623	6.2648720331
S15	2.5979584029	7.9810379438	5.0687640759
S16	3.3873771937	7.7830951031	8.4859331048
Mo17	4.7034261531	7.9125157692	6.4490696115
S18	6.6232744372	0.8009340489	5.4933374920
S19	5.1117077533	3.1556292950	4.4522745000
S20	5.7627536118	2.9127210763	7.4151554973
Mo21	7.3390587406	3.1516337746	5.5207369534
S22	5.2020959266	6.3997735692	4.6743563287
S23	5.8052434087	6.1092862785	7.6902814821
Mo24	7.3170315455	6.2643548249	5.7635388993
S25	4.2360067581	10.4064178285	6.4682696083
S26	9.5993615727	2.4188013411	4.8847467048
S27	7.6584846133	4.7925254201	3.7513906325
S28	8.4129326117	4.6246812062	7.1789942884
Mo29	9.5201847532	4.7263725602	5.1534231464
S30	7.0663616294	8.4998484612	6.7505897843
S31	9.6254122331	7.0100781616	5.0416490486
H32	7.4387031515	8.3959675961	8.3911966136
O33	4.4331369200	5.1912583395	11.7426029721
H34	4.8227164606	6.7135989126	11.6644402469
H35	4.3039057072	4.7798680381	12.6056804207
H36	5.1944416821	4.7261925172	11.3103934124

O37	6.6293672586	4.2942995585	10.5072053638
H38	6.4565561337	3.7785519915	9.7037406806
H39	7.0504792423	5.1135626218	10.2022885837
O40	5.1606484503	7.6459160374	11.4521544450
H41	4.5073150495	8.0219658540	10.8418542839
H42	6.3837033573	7.5360883227	10.8574613896
O43	7.3678413297	7.3798158390	10.4050872279
H44	7.4341988850	7.9767977155	9.3124994034
H45	8.0431479457	7.7645321592	10.9865662537

Heyrovsky transition state from **$[MoS_2]H_{Mo}^-$**

E = -9346.43704 Hartree

Mo1	1.8117211054	0.4483568936	5.7148009615
S2	-0.1619666823	1.4552995286	6.3591672802
Mo3	1.7228423145	3.0702847805	6.3975739168
S4	0.1407170176	4.7524490334	7.0991875041
Mo5	1.9180180509	6.4127689668	7.2104563156
S6	0.2192076120	8.0264693416	7.9738824830
Mo7	2.3013677912	9.0260458000	7.7767676841
S8	3.6141862135	-0.8168847153	5.0264308898
S9	2.3163784442	2.1563457105	4.2175549923
S10	2.9747863619	1.3104383253	7.5351944037
Mo11	4.2935064973	1.5227245528	5.4957006416
S12	2.4322231999	5.1036546774	5.1845979707
S13	2.9757279703	4.3612543556	8.0828161234
Mo14	4.5766041078	4.7129078324	6.2775079489
S15	2.7019521385	8.1424749057	5.6654056571
S16	3.2844945197	7.3212181779	9.0210076497
Mo17	4.6751003621	7.8876604797	7.0735963980

S18	6.5340081210	0.8892816025	4.8730235481
S19	5.1109123942	3.4952620203	4.2393587028
S20	5.7082570334	2.7219107456	7.1196744431
Mo21	7.3162481251	3.1618738715	5.2807178093
S22	5.3750674421	6.6679888430	5.0636907974
S23	5.8536663869	5.9116083896	7.9544758455
Mo24	7.5516548487	6.1606728228	6.1675060449
S25	4.2271988564	10.2593742198	7.8287818536
S26	9.4839163544	2.4293297222	4.4014637884
S27	7.7345202151	5.1448151546	3.9284588637
S28	8.4631600879	4.1361606893	7.1896498805
Mo29	9.6025422097	4.5984883505	5.2193680687
S30	6.8748205651	8.5762689607	6.6628619317
S31	9.9299357857	6.8356221585	5.4608150460
H32	8.5340056260	6.8513615814	7.5999258534
O33	5.1047061307	5.7786526795	11.5976586224
H34	6.0029749210	7.0769017197	11.2169672488
H35	4.9080622314	5.5950478681	12.5239393807
H36	5.6394115818	5.0162823844	11.2626168534
O37	6.8226609673	3.9776981255	10.5552063411
H38	6.4774091452	3.5252674992	9.7722099677
H39	7.5035961873	4.5864685103	10.2196549408
O40	6.6621824468	7.7454211604	10.8579963096
H41	6.1871734966	8.2743500020	10.2013750155
H42	7.7311624101	6.9863767575	10.2472420240
O43	8.4618160914	6.3628145473	9.8122771302
H44	8.4638895948	6.5950267226	8.4651181001
H45	9.3240466124	6.5992237594	10.1860031662

Tafel transition state from **$[MoS_2]H_5H_{Mo}$**

E = -9040.60869 Hartree

Mo1	1.7346738324	0.6391107158	6.9912095385
S2	-0.0220230330	1.8848359585	7.8437653293
Mo3	1.8774266892	3.3324466206	7.2260038618
S4	0.5451228970	5.2284297899	7.9491444418
Mo5	2.3439042239	6.7369488304	7.3959031463
S6	0.8688331581	8.5825739332	8.1426091006
Mo7	2.9081577018	9.3796237203	7.4278939329
S8	3.3106366517	-0.8349577427	6.1876180224
S9	1.9631633607	2.0496961705	5.1557182906
S10	3.2800480033	1.7008208053	8.3694117676
Mo11	4.1468176442	1.5057658081	6.1013365583
S12	2.3859874220	5.0912383771	5.5653826685
S13	3.5059371841	4.7945198298	8.3787342945
Mo14	4.6990290350	4.7576236691	6.2540555210
S15	2.8188493539	8.1413368129	5.4571050828
S16	4.1154164087	7.8379865070	8.6797992208
Mo17	5.0465567063	8.0276524167	6.4384497599
S18	6.1789125889	0.6287192893	5.1776048705
S19	4.7526776647	3.1904538536	4.3914012242
S20	5.9087744058	2.8562791964	7.1884711385
Mo21	7.1133303362	2.8767324181	5.0202559780
S22	5.2699174505	6.4307677346	4.5792510394
S23	6.3586107298	6.1453107891	7.3883792454
Mo24	7.6032243612	5.9282958945	5.2512896519
S25	4.7834749160	10.4993924306	6.7227296526
S26	9.0358520193	1.8297165971	3.9246211154
S27	7.3052144803	4.5179244587	3.2270656550

S28	8.6582063506	4.1235523838	6.4591185675
Mo29	9.3744717602	4.0974996142	4.2470205454
S30	7.1784554848	8.6417951516	5.4819092981
S31	9.8097222444	6.3157577947	4.0200739641
H32	8.1941530274	7.6265473628	6.1013803454
H33	8.7427618358	6.7288058955	6.3573442007

Reference

1. Jaramillo, T., Jørgensen, K., & Bonde, J. (2007). Science, 317(5834), 100–2.